**MIT-Palestine UROP Project**

Project title:

**Artificial Intelligence (AI) *En route* for Optimized Discovery of Drugs**

**Palestine Faculty**

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**MIT Faculty:**

Connor W. Coley, Assistant Professor

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**Co-PI:**

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Start date: Flexible

End date: Flexible

Estimated hours per week: 10-15

Application deadline

Website (if there is one for this project)

Required student skillset: Organic and Medicinal Chemistry, Pharmacology and Computer Skills. Familiarity with ChemDraw, chemical sketching and bioactivity, docking and virtual screening is advantageous.

Requested budget: None for the MIT end.

Requested budget for AQU: will be provided upon request.

Contacts: Connor W. Coley, Assistant Professor, Email: ccoley@mit.edu

**Overview**

Drug Discovery (DD) is rather a lengthy, complex and multistage process. The success rate among clinical candidates by responsible regulators like FDA and EMA is low when compared to the number of molecules make their way to preclinical and clinical phases. Its even more frustrating when considering the time, effort, and high investment in each candidate. Thus, AI emerges as fostering tool for increasing the success rate of clinical candidates. There are two main approaches applied so far in drug discovery: i) ligand-based and ii) structure-based. With the advancement computer-assisted drug discovery (CADD), sophisticated computational tools and modeling algorithms, availability of mega databases, (AI) is expected to contribute significantly in shaping the future landscape of drug discovery.

In this UROP-project, we aim at a) exploring modern computational tools employed in DD, b) got hands on in prominent methods allowing machine learning in DD c) training students and equip them with the ability to perform existing approaches and advanced techniques needed for prediction of molecular structure and function, and automated generation of innovative chemical entities with bespoke properties.